

# WANNIER FUNCTIONS OF ELLIPTIC ONE-GAP POTENTIAL

E D BELOKOLOS, V Z ENOLSKII, AND M SALERNO

**ABSTRACT.** Wannier functions of the one dimensional Schrödinger equation with elliptic one gap potential are explicitly constructed. Properties of these functions are analytically and numerically investigated. In particular we derive an expression for the amplitude of the Wannier function in the origin, a power series expansion valid in the vicinity of the origin and an asymptotic expansion characterising the decay of the Wannier function at large distances. Using these results we construct an approximate analytical expression of the Wannier function which is valid in the whole spatial domain and is in good agreement with numerical results.

## 1. INTRODUCTION

The spectral analysis of Schrödinger operators with periodic potentials has been investigated since the arbour of quantum mechanics. In spite of this, it still represents a non exhausted topic of ever continuing interest. From one side, it plays a fundamental role in condensed matter physics where it provides the mathematical basis of the quantum theory of solids. From the other, Schrödinger operators with periodic and quasi-periodic potentials play an important role in the integration of the Kortweg-de Vries (KdV) equation. Eigenstates of these operators, also called Bloch functions (BF), have been extensively studied during the past years by several authors (see [19, 2, 10]). An expression of the BF in terms of hyperelliptic  $\theta$ -functions was given in Ref. [12]. These studies were further developed in Ref. [15] where an algebro-geometric scheme for constructing solutions of non-linear equations was given in terms of the Baker–Akhiezer function. This function is uniquely defined on the Riemann surface associated with the energy spectrum and its properties are natural generalizations of the analytical properties of the BF of finite-gap potentials.

Besides BF, another set of functions which play an equally important role in condensed matter physics are the Wannier functions (WF) [16]. These functions are related to BF by a unitary transformation

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and form a complete set of localised orthonormal functions spanning a Bloch band. The properties of these functions were first investigated by Kohn in 1959 [13] in a classical paper in which the asymptotic decay of Wannier functions was characterised for the case of centrosymmetrical one-dimensional potentials. Since then, a large amount of work has been devoted to this topic and we mention here results only some of them. The projection operator technique was developed for construction of the Wannier functions and the Wannier functions were studied in the  $n$ -dimensional lattices [7], [8]. The localization problem for the Wannier functions was considered in a 1-dimensional case [6]. These functions were utilized with success in new practical methods for the electron energy calculation of solids (e.g. [14]) and in a number of modern calculation problems such as the photonic crystal circuits [4]. The Wannier functions represent the ideal basis for constructing effective Hamiltonians of quantum problems involving spatial localizations induced by electric and magnetic fields [17],[18], [11].

In spite of this, the properties of these functions are still not fully understood and, except for simplest cases, there are no models for which the analytical expression of the WF can be explicitly given. On the other hand, the recent results achieved in the field of completely integrable systems open the possibility to investigate analytical properties of the WF. Quite interestingly, WF have not been considered in the field of finite gap potentials.

The present paper represents a first contribution in this direction. In particular, we consider WF of Schrödinger operators with one-gap potentials and use the well developed theory of elliptic functions to investigate their properties with sufficient completeness. As a result we derive: *i*) an exact value for the amplitude of the WF at the localization site; *ii*) an asymptotic expansion characterising the decay of the WF at large distances; *iii*) a power series expansion valid in the vicinity of the localization site. Using results *ii*), *iii*), we construct an approximate analytical representation of the WF which is valid in the whole spatial domain. These results are shown to be in very good agreement with the WF obtained by means of numerical methods.

The paper is organised as follows. In Section 2 we discuss the basic properties of the BF for one gap potentials. In particular we introduce basic definitions, discuss the basic properties of BF and derive the analytical expression of their normalization constants. Section 3 is devoted to the study of the WF. After recalling the basic definitions we derive the main results of the paper i.e. points *i*)-*iii*) listed above. In Section 4 we construct an approximate analytical expression of the WF and compare the results of our theory with WF obtained from the basic

definition using numerical tools. Finally, in Section 5 we summarise the main results of the paper and briefly discuss future developments.

## 2. PROPERTIES OF BLOCH FUNCTIONS OF ONE-GAP POTENTIAL

**2.1. The Schrödinger equation with one-gap potential.** In the paper we use standard notations and facts of the theory of elliptic functions. In particular we use the well known Weierstrass  $\wp$ -,  $\sigma$ - and  $\zeta$ -functions.

The periodic elliptic one-gap potential  $\mathcal{U}(x)$  considered in this paper, is expressed in terms of the Weierstrass  $\wp$ -function as

$$(2.1) \quad \begin{aligned} \mathcal{U}(x) &= -2\wp(u), \quad u = ix + \omega, \quad x \in \mathbb{R}, \\ \mathcal{U}(x + nT) &= \mathcal{U}(x), \quad n \in \mathbb{N}, \end{aligned}$$

where  $T = -2i\omega'$  is the period of the lattice (notice that  $T$  is real and  $\mathcal{U}(x) = 2\wp(ix + \omega)$  is a smooth periodic real function). The Schrödinger equation associated with potential (2.1)

$$(2.2) \quad \partial_x^2 \Psi(x; E) + (E - \mathcal{U}(x))\Psi(x; E) = 0.$$

As is well known (see for example [3] and references therein), this equation admits eigenfunctions  $\Psi(x; E)$  which satisfy the Bloch condition

$$(2.3) \quad \Psi(x - T; E) = e^{-ik(E)T} \Psi(x; E),$$

where  $E$  is the energy given by

$$(2.4) \quad E = \wp(v), \quad v = \alpha + \omega', \quad \alpha \in \mathbb{R},$$

and  $k(E)$  is the quasi-momentum given by

$$(2.5) \quad k(v) = \zeta(v) - \frac{\eta'}{\omega'}v, \quad v = \alpha + \omega', \quad \alpha \in \mathbb{R}.$$

Eigenfunctions of type (2.3) are called Bloch functions. Notice that the dependence of the quasi-momentum on the energy (and vice versa) arises from the elimination of the parameter  $\alpha$  from Eqs. (2.4), (2.5). The BF can be written in explicit form as

$$(2.6) \quad \Psi(u; v) = C(v) \frac{\sigma(v - u)}{\sigma(v)\sigma(u)} \exp\{u\zeta(\alpha)\},$$

or, alternatively, as

$$(2.7) \quad \Psi(u, v) = D(v) \sqrt{\wp(u) - \wp(v)} \exp \left\{ \frac{\wp'(v)}{2} \int^x \frac{du}{\wp(u) - \wp(v)} \right\},$$

where  $C(v), D(v)$  are proper normalization constants. In the following we shall use both representations for the BF. Notice that the BF considered as function of  $k$  instead of  $\alpha$ , is periodic in the reciprocal space, with period

$$2\tilde{\omega} = \frac{i\pi}{\omega'}.$$

BF has the following following periodicity properties

(2.8)

$$\Psi(u + 2n\omega; v) = \exp\{2n\omega k(v)\} \Psi(u; v), \quad k(v) = \zeta(v) - v \frac{\eta}{\omega},$$

(2.9)

$$\Psi(u + 2n'\omega'; v) = \exp\{2n'\omega' k'(v)\} \Psi(u; v), \quad k'(v) = \zeta(v) - v \frac{\eta'}{\omega'}.$$

**2.2. Normalization of the Bloch function of one-gap potentials.** Since the normalization of the BF plays an important role in the construction of the WF (see next section), we shall show how to compute the normalization constant, although this question has been considered in Chapt. VIII of [2].

We normalise the BF according to

$$(2.10) \quad 2\pi \langle |\Psi(x, E)|^2 \rangle = 1,$$

where

$$\langle f(x) \rangle = \lim_{L \rightarrow \infty} \frac{1}{L} \int_{-\frac{1}{2}L}^{\frac{1}{2}L} f(x) dx.$$

The following proposition is valid.

**Proposition 2.1.** *Normalised Bloch functions of elliptic one-gap potentials are of the form*

(2.11)

$$\Psi(x; \alpha) = -\frac{i}{(2\pi)^{1/2}} \left[ -\wp(v) - \frac{\eta'}{\omega'} \right]^{-1/2} \frac{\sigma(v-u)}{\sigma(v)\sigma(u)} \exp\{v\eta + (u-\omega)\zeta(v)\},$$

where  $u = ix + \omega$ ,  $x \in \mathbb{R}$ ;  $v = \alpha + \omega'$ ,  $\alpha \in \mathbb{R}$ .

*Proof.* Let us denote the normalised BF as

$$\Psi(u; v) = C(v) \Phi(u; v),$$

where  $\Phi(u; v)$  is the non-normalised BF

$$\Phi(u; v) = \frac{\sigma(v-u)}{\sigma(v)\sigma(u)} e^{(u-\omega)\zeta(v)},$$

and  $C(v)$  is the normalization constant defined by Eq. (2.10)

$$2\pi \frac{|C(v)|^2}{2\omega'} \int_{\omega}^{\omega+2\omega'} |\Phi(u; v)|^2 du = 1.$$

The complex conjugated (non-normalised) BF is

$$\begin{aligned} \overline{\Phi}(u; v) &= \frac{\overline{\sigma}(v-u)}{\overline{\sigma}(v)\overline{\sigma}(u)} e^{-(u-\omega)\overline{\zeta}(v)} = \frac{\sigma(\overline{v}-\overline{u})}{\sigma(\overline{v})\sigma(\overline{u})} e^{-(u-\omega)\zeta(\overline{v})} \\ &= -\frac{\sigma(v-2\omega'+u-2\omega)}{\sigma(v-2\omega')} \sigma(u-2\omega) e^{(u-\omega)\zeta(v-2\omega')} \\ &= \frac{\sigma(v+u)}{\sigma(v)\sigma(u)} e^{-(v-\omega')2\eta-(u-\omega)\zeta(v)}, \end{aligned}$$

where the following elementary equalities were used

$$\begin{aligned} \overline{\sigma}(z) &= \sigma(\overline{z}), \quad \overline{\zeta}(z) = \zeta(\overline{z}), \quad \overline{(u-\omega)} = -(u-\omega), \\ \overline{u} &= -u+2\omega, \quad \overline{v} = v-2\omega', \\ \zeta(v-2\omega') &= \zeta(v) - 2\eta', \\ \sigma(v-2\omega') &= -\sigma(v) \exp(-(v-\omega')2\eta'), \\ \sigma(u-2\omega) &= -\sigma(u) \exp(-(u-\omega)2\eta). \end{aligned}$$

By multiplying the above expressions of  $\Phi(u; v)$  and  $\overline{\Phi}(u; v)$  we get

$$|\Phi(u; v)|^2 = \frac{\sigma(v-u)\sigma(v+u)}{\sigma^2(v)\sigma^2(u)} e^{-(v-\omega')2\eta} = [\wp(u) - \wp(v)] e^{(v-\omega')2\eta},$$

where in the last step we have used the well known formula

$$\frac{\sigma(v-u)\sigma(v+u)}{\sigma^2(v)\sigma^2(u)} = \wp(u) - \wp(v).$$

The normalization condition can be then written in the form

$$\begin{aligned} 1 &= 2\pi \frac{|C(v)|^2}{2\omega'} \int_{\omega}^{\omega+2\omega'} [\wp(u) - \wp(v)] e^{(v-\omega')2\eta} du \\ &= 2\pi |C(v)|^2 \left[ -\frac{\eta'}{\omega'} - \wp(v) \right] e^{-(v-\omega')2\eta}, \end{aligned}$$

since

$$\frac{1}{2\omega'} \int_{\omega}^{\omega+2\omega'} \wp(u) du = \frac{1}{2\omega'} [\zeta(\omega) - \zeta(\omega+2\omega')] = -\frac{\eta'}{\omega'}.$$

Thus we have obtained for the normalization constant the expression

$$(2.12) \quad C(v) = \frac{e^{i\theta}}{(2\pi)^{1/2}} \left[ -\frac{\eta'}{\omega'} - \wp(v) \right]^{-1/2} e^{(v-\omega')\eta},$$

with an arbitrary phase factor  $\exp(i\theta)$ ,  $\theta \in \mathbb{R}$ . In the following we fix this factor as

$$\exp(i\theta) = \exp(\omega'\eta - i(\pi/2)).$$

□

The normalised BF,  $\Psi(u; v)$ , satisfy a number of useful properties under the action of symmetry operations. For centro-symmetrical potentials the transformation  $x \rightarrow -x$  of the lattice corresponds to a transformation in the Jacobian  $u \rightarrow \hat{u} = -u + 2\omega$ , and the following propositions can be proved.

**Proposition 2.2.**

$$\Psi(\hat{u}; v) = \Psi(-u + 2\omega; v) = \overline{\Psi}(u; v).$$

*Proof.*

$$\begin{aligned} \Psi(\hat{u}; v) &= \Psi(-u + 2\omega; v) \\ &= i(2\pi)^{-1/2} \left[ -\wp(v) - \frac{\eta'}{\omega'} \right]^{-1/2} \frac{\sigma(v+u-2\omega)}{\sigma(v)\sigma(u-2\omega)} \exp[v\eta - (u-\omega)\zeta(v)] \\ &= i(2\pi)^{-1/2} \left[ -\wp(v) - \frac{\eta'}{\omega'} \right]^{-1/2} \frac{\sigma(v+u)}{\sigma(v)\sigma(u)} \exp[-v\eta - (u-\omega)\zeta(v)] = \overline{\Psi}(u; v). \end{aligned}$$

□

Similarly, that the transformation  $\alpha \rightarrow -\alpha$  corresponds to  $v \rightarrow \hat{v} = -v + 2\omega'$ , and the following proposition is valid.

**Proposition 2.3.**

$$\Psi(u; \hat{v}) = \Psi(u; -v + 2\omega') = \overline{\Psi}(u; v).$$

*Proof.*

$$\begin{aligned} \Psi(u; \hat{v}) &= \Psi(u; -v + 2\omega') \\ &= -i(2\pi)^{-1/2} \left[ -\wp(v) - \frac{\eta'}{\omega'} \right]^{-1/2} \frac{\sigma(-v-u+2\omega')}{\sigma(-v+2\omega')\sigma(u)} \\ &\quad \times \exp[(-v+2\omega')\eta + (u-\omega)\zeta(v-2\omega')] \\ &= -i(2\pi)^{-1/2} \left[ -\wp(v) - \frac{\eta'}{\omega'} \right]^{-1/2} \frac{\sigma(v+u)}{\sigma(v)\sigma(u)} \exp[-v\eta - (u-\omega)\zeta(v)] \\ &= \overline{\Psi}(u; v). \end{aligned}$$

□

The above propositions can be used to study the elementary properties of the BF,  $\Psi(x; k) \equiv \Psi(u(x); v(k))$ , where  $u(x) = ix + \omega$  and  $v(k)$  is the inverse of the function  $k(v) = \zeta(v) - (\eta'/\omega')v$ . To this regard note that

$$x(\hat{u}) = -x(u), \quad k(\hat{v}) = -k(v).$$

The following two properties are easily proved.

**Property 1.**  $\Psi(-x; k) = \overline{\Psi}(x; k)$ ,

*Proof.*

$$\Psi(-x; k) = \Psi(\hat{u}, v) = \overline{\Psi}(u; v) = \overline{\Psi}(x; k);$$

□

**Property 2.**  $\Psi(x; -k) = \overline{\Psi}(x; k)$ ,

*Proof.*

$$\Psi(x; -k) = \Psi(u; \hat{v}) = \overline{\Psi}(u; v) = \overline{\Psi}(x; k).$$

□

### 3. ANALYTICAL PROPERTIES OF THE WANNIER FUNCTION OF ELLIPTIC ONE-GAP POTENTIALS

**3.1. Definition and basic properties.** In 1937 G. Wannier introduced a complete set of functions for an electron in a lattice structure [16]. The Wannier functions,  $W_n(x)$ , are defined as

$$(3.1) \quad W_n(x) = \left( \frac{T}{2\pi} \right)^{1/2} \int_{-\pi/T}^{\pi/T} \Psi_n(x; k) dk.$$

where the integral is made on the Brillouin zone. WF for the Schrödinger operator with periodic potential  $U(x), U(x - mT), m \in \mathbb{Z}$  are localised linear combinations of all the Bloch eigenstates of a given  $n$ -th spectral band. One can easily prove that if the BF is normalised according to Eq. (2.10), then the WF is normalised on the full line,

$$\int_{-\infty}^{\infty} |W_n(x)|^2 dx = 1.$$

Using the translation operator one then constructs a countable set of WF:  $W_n^{(l)}(x) := W_n(x - lT)$ ,  $l \in \mathbb{Z}$  which is complete and forms an ortho-normal basis

$$\int_{-\infty}^{\infty} \overline{W}_n^{(l)}(x) W_{n'}^{(l')}(x) dx = \delta_{nn'} \delta_{ll'}, \quad l \in \mathbb{Z}.$$

The inverse transformation allows to express a BF in terms of WF as

$$(3.2) \quad \Psi_n(x; k) = \left(\frac{T}{2\pi}\right)^{1/2} \sum_{l=-\infty}^{\infty} W_n^{(l)}(x) e^{ilak}.$$

In the following we shall omit the band index  $n$  since we deal only with one band. Properties of WF of one dimensional periodic potentials were studied by W. Kohn [13] where he proved that for every band there exists one and only one WF which satisfies simultaneously the following three properties 1)  $\overline{W}(x) = W(x)$ ; 2)  $W(-x) = \pm W(x)$ ; 3)  $W(x) = O(\exp(-h|x|))$ , where  $h > 0$ . In the following we investigate the analytical properties of the WF for the one-gap potential in Eq. (2.1). In this case the WF is given by the formula

$$\begin{aligned} W(x) &= \left(\frac{T}{2\pi}\right)^{1/2} \int_{-\pi/T}^{\pi/T} \Psi(x; k) dk \\ &= \left(\frac{T}{2\pi}\right)^{1/2} \left( \int_{-\pi/T}^0 + \int_0^{\pi/T} \right) \Psi(x; k) dk \\ &= \left(\frac{T}{2\pi}\right)^{\frac{1}{2}} \int_0^{\pi/T} (\Psi(x; k) + \Psi(x; -k)) dk \\ &= \left(\frac{T}{2\pi}\right)^{1/2} 2\operatorname{Re} \int_0^{\pi/T} \Psi(x; k) dk \\ (3.3) \quad &= \operatorname{Re} \left\{ -i \frac{\sqrt{-2i\omega'}}{\pi} \int_{\omega'}^{\omega+\omega'} \sqrt{\frac{dk(v)}{dv}} \frac{\sigma(v-u)}{\sigma(v)\sigma(u)} e^{v\eta+(u-\omega)\zeta(v)} dv \right\}. \end{aligned}$$

Using the properties of the BF,  $\Psi(x; k)$ , the following basic properties of the WF can be proved.

**Proposition 3.1.**  $\overline{W}(x) = W(x)$ .

*Proof.*

$$\begin{aligned} \overline{W}(x) &= \left(\frac{2T}{\pi}\right)^{1/2} \operatorname{Re} \int_0^{\pi/T} \overline{\Psi}(x; k) dk \\ &= \left(\frac{2T}{\pi}\right)^{1/2} \operatorname{Re} \int_0^{\pi/T} \Psi(x; k) dk = W(x). \end{aligned}$$

□

**Proposition 3.2.**  $W(-x) = W(x)$ .



*Proof.*

$$\begin{aligned} W(-x) &= \left(\frac{2T}{\pi}\right)^{1/2} \operatorname{Re} \int_0^{\pi/T} \Psi(-x; k) dk = \left(\frac{2T}{\pi}\right)^{1/2} \operatorname{Re} \int_0^{\pi/T} \overline{\Psi}(x; k) dk \\ &= \left(\frac{2T}{\pi}\right)^{1/2} \operatorname{Re} \int_0^{\pi/T} \Psi(x; k) dk = W(x). \end{aligned}$$

□

### 3.2. Power series expansion of the Wannier function at $x=0$ .

We shall construct in this section the power series expansion of the Wannier function of one gap potential.

**Theorem 3.3.** *The Wannier function of the lower energy band for the one gap potential admits the following power series representation*

$$(3.4) \quad W(x) = \sum_{p=0}^{\infty} \frac{(-1)^p}{(2p)!} W_{2p} x^{2p},$$

where the coefficients  $W_{2p}$  of the expansion (3.4) are given by the formula

$$(3.5) \quad W_{2p} = \sum_{l=0}^p M_l q_{p,l}.$$

Here

$$(3.6) \quad \begin{aligned} M_l &= \frac{\sqrt{2i}}{\pi} \sqrt{\omega' e_3 + \eta'} \sum_{j=0}^l \frac{(2j-1)!! l!}{2^j (j!)^2 (l-j)!} e_3^j (e_2 - e_3)^{l-j} \\ &\quad \times F\left(-\frac{1}{2}, j + \frac{1}{2}; j + 1; \frac{\omega'(e_3 - e_2)}{\omega' e_3 + \eta'}\right), \end{aligned}$$

where  $F(a, b; c; z)$  is the standard hypergeometric function,  $e_2, e_3$  are branch points of the elliptic curve and  $q_{p,l}$  are coefficients of polynomials in  $\wp(v)$

$$Q_p(\wp(v)) = \sum_{l=0}^p q_{p,l} \wp^l(v)$$

defined by the recurrence

$$(3.7) \quad Q_p(\wp(v)) = \sum_{m=0}^{p-1} \binom{2p}{2m-2} \phi_{m-p-1} Q_m(\wp(v))$$

with

$$\phi_0 = 2e_1 + \wp(v), \quad \phi_p = 2\wp^{(2p)}(\omega).$$

First few coefficients of the expansion (3.4) are

$$\begin{aligned}
 W_0 &= M_0, \\
 W_2 &= M_1 + 2e_1 M_0, \\
 (3.8) \quad W_4 &= M_2 + 4e_1 M_1 + (4e_1^2 + 2\wp''(\omega))M_0, \\
 W_6 &= M_3 + 6e_1 M_2 + (14\wp''(\omega) + 12e_1^2)M_1 \\
 &\quad + (2\wp^{(IV)}(\omega) + 28\wp''(\omega)e_1 + 8e_1^3)M_0.
 \end{aligned}$$

*Proof.* We have

$$(3.9) \quad W(x) = \left(\frac{2T}{\pi}\right)^{\frac{1}{2}} \operatorname{Re} \int_0^{\pi/T} \Psi(x; k) dk.$$

Because the BF  $\Psi(x; k)$  is even in  $x$  we can write it in the form of Taylor expansion

$$(3.10) \quad \Psi(u, v) = \sum_{p=0}^{\infty} \frac{(-1)^p}{(2p)!} \Psi_{2p}(v) x^{2p},$$

where

$$\Psi_{2p}(v) = \left[ \frac{d^{2p}}{du^{2p}} \Psi(u, v) \right]_{u=\omega}, \quad p = 1, \dots$$

If we substitute the Taylor expansion (3.10) to the (3.9) we obtain the expansion (3.4) with the following coefficients

$$(3.11) \quad W_{2p} = \left(\frac{2T}{\pi}\right)^{1/2} \operatorname{Re} \int_0^{\pi/T} \Psi_{2p}(v) dk.$$

Using Schrödinger equation we obtain easily for the  $\Psi_{2p}(v)$  a recurrent relation

$$\begin{aligned}
 \Psi_{2p}(v) &= \sum_{l=0}^{p-1} \binom{2p}{2l-2} \phi_{p-l-1} \Psi_{2l}(v) \\
 \phi_0 &= 2e_1 + \wp(v), \quad \phi_p = 2\wp^{(2p)}(\omega).
 \end{aligned}$$

The form of this relation leads to conclusion that

$$\Psi_{2p}(v) = Q_p(\wp(v)) \Psi_0(v),$$

where

$$(3.12) \quad \Psi_0(v) = \Psi(\omega; v) = \frac{1}{\sqrt{2\pi}} \sqrt{\frac{\wp(v) - e_1}{\wp(v) + \frac{\eta'}{\omega'}}$$

and  $Q_p(\wp(v))$  are polynomials of the  $p$ -th order in  $\wp(v)$ ,

$$Q_p(\wp(v)) = \sum_{l=0}^p q_{p,l} \wp^l(v).$$

Similarly to  $\Psi_{2p}(v)$  the polynomials  $Q_p(\wp(v))$  satisfy the following recurrent relation

$$(3.13) \quad Q_p(\wp(v)) = \sum_{m=0}^{p-1} \binom{2p}{2m-2} \phi_{m-p-1} Q_m(\wp(v))$$

with

$$\phi_0 = 2e_1 + \wp(v), \quad \phi_p = 2\wp^{(2p)}(\omega).$$

In particular the first few polynomials  $Q_p(\wp(v))$  are

$$(3.14) \quad \begin{aligned} Q_1(\wp(v)) &= \wp(v) + 2e_1, \\ Q_2(\wp(v)) &= \wp(v)^2 + 4e_1\wp(v) + 2\wp''(\omega) + 4e_1^2, \\ Q_3(\wp(v)) &= \wp(v)^3 + 6e_1\wp(v)^2 + (14\wp''(\omega) + 12e_1^2)\wp(v) \\ &\quad + 2\wp^{(IV)}(\omega) + 28e_1\wp''(\omega) + 8e_1^3. \end{aligned}$$

Next we calculate the integral expressions of the coefficients  $W_{2p}$ . We show that the following formula is valid

$$\begin{aligned} M_l &= -2 \left( \frac{\omega'}{i\pi} \right)^{1/2} \int_0^{\omega'} \wp(v)^l \left( \wp(v) + \frac{\eta'}{\omega'} \right) \Psi(\omega; v) dv \\ &= \left( \frac{2T}{\pi} \right)^{\frac{1}{2}} \int_0^{\omega'} \wp(v)^l \frac{1}{\sqrt{2\pi}} \sqrt{\frac{\wp(v) - e_1}{\wp(v) + \frac{\eta'}{\omega'}}} \left( -\wp(v) - \frac{\eta'}{\omega'} \right) dv \\ &= \frac{T^{\frac{1}{2}}}{\pi} \int_0^{\omega'} \wp(v)^l \sqrt{\wp(v) - e_1} \sqrt{\wp(v) + \frac{\eta'}{\omega'}} dv. \end{aligned}$$

After the substitution  $\wp(v) = s$ , the computation is reduced to the derivation of the complete elliptic integral

$$(3.15) \quad M_l = -\frac{\sqrt{-i\omega'}}{\pi} \int_{e_3}^{e_2} s^l \sqrt{\frac{s + \frac{\eta'}{\omega'}}{(s - e_2)(s - e_3)}} ds.$$

By introducing the new variable

$$t = \frac{s - e_3}{e_2 - e_3},$$

the integral  $M_l$  acquires the form

$$(3.16) \quad M_l = -\frac{\sqrt{-i\omega'}}{\pi} \sqrt{e_2 - e_3} \int_0^1 ((e_2 - e_3)t - e_3)^l \sqrt{\frac{1 - \tilde{k}^2 t}{t(1-t)}} dt,$$

where

$$(3.17) \quad \tilde{k} = \sqrt{\frac{\omega'(e_3 - e_2)}{\omega'e_3 + \eta'}},$$

is the Jacobi modulus of the elliptic curve

$$(3.18) \quad Y^2 = (X - e_2)(X - e_3) \left( X + \frac{\eta'}{\omega'} \right).$$

Using the integral representation of the hypergeometric function (see e.g. [1])

$$(3.19) \quad F(a, b; c; z) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_0^1 \frac{t^{b-1}(1-t)^{c-b-1}}{(1-tz)^a} dt,$$

we obtain the required expression

$$(3.20) \quad M_l = \frac{\sqrt{2i}}{\pi} \sqrt{\omega'e_3 + \eta'} \sum_{j=0}^l \frac{(2j-1)!!!}{2^j(j!)^2(l-j)!} e_3^j (e_2 - e_3)^{l-j} \times F\left(-\frac{1}{2}, j + \frac{1}{2}; j + 1; \tilde{k}^2\right).$$

□

It is worth to note that the coefficient  $W_0$  gives an exact value of the amplitude of WF at the localization site  $x = 0$ ,

$$(3.21) \quad W_0 = \frac{\sqrt{2i}}{2} \sqrt{\omega'e_3 + \eta'} F\left(-\frac{1}{2}, \frac{1}{2}; 1; \tilde{k}^2\right).$$

This amplitude can also be written in the alternative form

$$(3.22) \quad W_0 = \frac{\sqrt{2i}}{\pi} \sqrt{\omega'e_3 + \eta'} E(\tilde{k}),$$

where  $E(\tilde{k})$  is the complete integral of the second kind depending on  $\tilde{k}$ . Also note that by using the relations

$$\begin{aligned} \left( z \frac{d}{dz} + b \right) &= b F(a, b+1; c; z), \\ \left[ (1-z) \frac{d}{dz} + c - a - b \right] F(a, b; c; z) &= \frac{(c-a)(c-b)}{c} F(a, b; c+1; z), \end{aligned}$$

one can express all hyperegeometric functions  $F(-\frac{1}{2}, j + \frac{1}{2}; j + 1; \tilde{k}^2)$  in (3.20) in terms of the derivatives of  $F(-\frac{1}{2}, \frac{1}{2}; 1; \tilde{k}^2)$  with respect to  $\tilde{k}^2$ , and therefore the whole expression can be written in terms of the complete integral  $E(\tilde{k})$  and of its derivatives.

We remark that the quantities  $\wp^{(2j)}(\omega), j = 1, \dots$ , can be computed in recurrent way, the some first of them are [1]

$$\begin{aligned}\wp''(\omega) &= 3! \left( e_1^2 - \frac{1}{2^2 \cdot 3} g_2 \right), \\ \wp^{(IV)}(\omega) &= 5! \left( e_1^3 - \frac{3}{2^2 \cdot 5} g_2 e_1 - \frac{1}{2 \cdot 5} g_3 \right), \\ \wp^{(VI)}(\omega) &= 7! \left( e_1^4 - \frac{1}{5} g_2 e_1^2 - \frac{1}{7} g_3 e_1 + \frac{1}{2^4 \cdot 5 \cdot 7} g_2^2 \right).\end{aligned}$$

**3.3. Asymptotic expansion of the Wannier function.** In this section we obtain the asymptotic expression for the WF at  $x \rightarrow +\infty$  by the steepest descent method. This method (see, e.g. [9]) permits to compute the asymptotic expression of integrals of the type

$$F(x) = \int_{\gamma} f(z) \exp\{xS(z)\} dz,$$

where  $\gamma$  is a contour in the complex plane and the functions  $f(z)$  and  $S(z)$  are holomorphic in the vicinity of  $\gamma$ . When a saddle point  $z_0$ , which is defined by the equation

$$\frac{d}{dz} S(z_0) = 0,$$

does not coincide with the edges of the contour, the asymptotic formula of the integral  $F(x)$  reads

$$F(x) = \sqrt{-\frac{2\pi}{x \frac{d^2 S(z_0)}{dz^2}}} \exp\{xS(z_0)\} [f(z_0) + O(x^{-1})].$$

In our case we must use a non-standard variant of the steepest descents method, since the exponential in the integrand will have the form  $xS(z)$  only at  $|x| \rightarrow +\infty$  and  $f(z_0) = 0$ .

**Proposition 3.4.** *At  $x \rightarrow \infty$  the Wannier function of the lower energy band for the one gap potential has the following asymptotic expression (3.23)*

$$W(x) \simeq \operatorname{Re} \left\{ \frac{\sqrt{-2i\omega'}}{\pi} \left( e_1 + \frac{\eta'}{\omega'} \right)^{1/2} \frac{\sigma(v-u)}{\sigma(v)\sigma(u)} e^{(u-\omega)\zeta(v)} \left[ \frac{i}{2\wp'(v)} \right]^{1/4} \frac{\Gamma(\frac{3}{4})}{x^{\frac{3}{4}}} \right\},$$

where  $v$  is a solution of the equation

$$(3.24) \quad \wp(v) = -\frac{\eta'}{\omega'}, \quad \text{or} \quad k'(v) = 0,$$

such that the complex number  $\omega'k(v) = \omega'(\zeta(v) - (\eta'/\omega')v)$  has negative real part. This means that

$$W(x) \simeq \exp(-h|x|)|x|^{-3/4}, \quad |x| \rightarrow \infty,$$

where  $h = |k(v)|$  and  $v$  is defined by the equation  $k'(v) = 0$ .

*Proof.* We use the expression of the WF for the first energy band  $[e_3, e_2]$  given in Eq. (3.3). Since

$$\begin{aligned} \frac{\sigma(v-u)}{\sigma(v)\sigma(u)} &= -\frac{\sigma(u-v)}{\sigma(\omega-v)} \frac{\sigma(\omega)}{\sigma(u)} \frac{\sigma(\omega-v)}{\sigma(v)\sigma(\omega)} \\ &= \frac{\sigma(v-\omega)}{\sigma(v)\sigma(\omega)} \exp \left\{ \int_{\omega}^u [\zeta(s-v) - \zeta(s)] ds \right\} \\ &= [\wp(v) - e_1]^{1/2} \exp \left\{ -v\eta + \int_{\omega}^u [\zeta(s-v) - \zeta(s)] ds \right\}, \end{aligned}$$

we have that Eq. (3.3) can be rewritten as

$$(3.25) \quad W(x) = \operatorname{Re} \left\{ \frac{\sqrt{-2i\omega'}}{\pi} \int_{\omega'}^{\omega+\omega'} [e_1 - \wp(v)]^{1/2} \sqrt{\frac{dk(v)}{dv}} \right. \\ \left. \times \exp \left\{ \int_{\omega}^u [\zeta(s-v) - \zeta(s) + \zeta(v)] ds \right\} dv \right\}.$$

When  $x \rightarrow +\infty$  we can calculate the integral in Eq. (3.25) by the steepest descents method. To this regard we remark that the argument of the exponential, as a function of  $v$ , has saddle points which are defined by the equation

$$\frac{d}{dv} \int_{\omega}^u [\zeta(s-v) - \zeta(s) + \zeta(v)] ds = 0,$$

or, in other words, by the equation

$$\wp(v) = -\frac{\zeta(u-v) - \zeta(\omega-v)}{u-\omega}.$$

At  $x \rightarrow +\infty$  the last equation attains the form (3.24). Since  $\overline{\wp}(v) = \wp(\overline{v})$  we have that if  $v$  is saddle point then  $\overline{v}$  is also a saddle point. On the other hand,  $\wp(v)$  is an elliptic function of the second order, so it takes every value twice in the fundamental domain, this implying that there are two saddle points, say  $v_1, v_2$ , in the fundamental domain. The

sum of the values  $v_1, v_2$  must be a period of the lattice, which in our case means that  $v_1 + v_2 = 2(\omega + \omega')$ . It is not difficult to show that

$$v_1 = \omega + \omega' + i\beta, \quad v_2 = \omega + \omega' - i\beta, \quad \beta \in \mathbb{R},$$

i.e. the two saddle points  $v_1, v_2$ , are situated in the spectral gap. The periodicity of the Weierstrass function  $\wp(z)$  in the complex plane give rise to countable set  $V$  of saddle points,

$$V = \{v_1 + 2n_1\omega', v_2 + 2n_2\omega' : n_1, n_2 \in \mathbb{Z}\}.$$

In order to build the proper asymptotic expression for the Wannier function  $W(x)$  we must select from this set a special saddle point which we denote by  $v_0$ . In the neighbourhood of  $v_0$  we have

$$\sqrt{\frac{dk(v)}{dv}} \simeq [-\wp'(v_0)]^{1/2}(v - v_0)^{1/2},$$

$$\begin{aligned} & \int_{\omega}^u [\zeta(s - v) - \zeta(s) + \zeta(v)] ds \simeq \int_{\omega}^u [\zeta(s - v_0) - \zeta(s) + \zeta(v_0)] ds \\ & + \frac{1}{2}(v - v_0)^2 \int_{\omega}^u [\zeta''(s - v_0) + \zeta''(v_0)] ds = \int_{\omega}^u [\zeta(s - v_0) - \zeta(s) + \zeta(v_0)] ds \\ & - (u - \omega) \frac{1}{2} \left[ \wp'(v_0) + \frac{\wp(u - v_0) - \wp(\omega - v_0)}{u - \omega} \right] (v - v_0)^2 \\ & \simeq \int_{\omega}^u [\zeta(s - v_0) - \zeta(s) + \zeta(v_0)] ds - (u - \omega) \frac{1}{2} \wp'(v_0) (v - v_0)^2. \end{aligned}$$

Substituting the last two expressions into the integral representation of the WF in (3.25), we obtain

$$\begin{aligned} W_0(x) & \simeq \operatorname{Re} \left\{ \frac{\sqrt{-2i\omega'}}{\pi} \left( e_1 + \frac{\eta'}{\omega'} \right)^{1/2} \exp \left\{ \int_{\omega}^u [\zeta(s - v_0) - \zeta(s) + \zeta(v_0)] ds \right\} \right. \\ & \times \left. \int_{C_0} dv [-\wp'(v_0)]^{1/2} (v - v_0)^{1/2} \exp \left\{ -\frac{1}{2}(u - \omega) \wp'(v_0) (v - v_0)^2 \right\} \right\} \\ & = \operatorname{Re} \left\{ \frac{\sqrt{-2i\omega'}}{\pi} \left( e_1 + \frac{\eta'}{\omega'} \right)^{1/2} \frac{\sigma(v_0 - u)}{\sigma(v_0)\sigma(u)} \exp \{ (u - \omega) \zeta(v_0) \} \right. \\ & \times \left. \int_{C_0} dr [-\wp'(v_0)]^{1/2} r^{1/2} \exp \left\{ -\frac{1}{2}(u - \omega) \wp'(v_0) r^2 \right\} \right\}, \end{aligned}$$

where  $C_0$  is a contour passing through the saddle point  $v_0$ . The integral in the last expression can be calculated as

$$\begin{aligned} I_0 &= \int_{C_0} dr [-\wp'(v_0)]^{1/2} r^{1/2} \exp \left\{ -\frac{1}{2}(u - \omega) \wp'(v_0) r^2 \right\} \\ &= \left[ \frac{i}{2\wp'(v_0)} \right]^{1/4} \frac{1}{x^{3/4}} \int_0^\infty e^{-t} t^{-1/4} dt = \left[ \frac{i}{2\wp'(v_0)} \right]^{1/4} \frac{\Gamma(\frac{3}{4})}{x^{3/4}}. \end{aligned}$$

Notice that, since  $\wp'(v_0) = -2[\wp(v_0) - e_1]^{1/2}[\wp(v_0) - e_2]^{1/2}[\wp(v_0) - e_3]^{1/2}$ , and  $e_3 \leq e_2 \leq \wp(v_0) \leq e_1$ , we have that  $\wp'(v_0) = -i|\wp'(v_0)|$ .

For the function  $W_0(x)$  we finally obtain

$$\begin{aligned} W_0(x) &\simeq \operatorname{Re} \left\{ \frac{\sqrt{-2i\omega'}}{\pi} \left( e_1 + \frac{\eta'}{\omega'} \right)^{1/2} \left[ \frac{i}{2\wp'(v_0)} \right]^{1/4} \frac{\Gamma(\frac{3}{4})}{x^{3/4}} \right. \\ &\quad \times \exp \left\{ \int_\omega^u [\zeta(s - v_0) - \zeta(s) + \zeta(v_0)] ds \right\} \Big\} \\ &= \operatorname{Re} \left\{ \frac{\sqrt{-2i\omega'}}{\pi} \left( e_1 + \frac{\eta'}{\omega'} \right)^{1/2} \frac{\sigma(v_0 - u)}{\sigma(v_0)\sigma(u)} e^{(u - \omega)\zeta(v_0)} \left[ \frac{i}{2\wp'(v_0)} \right]^{1/4} \frac{\Gamma(\frac{3}{4})}{x^{3/4}} \right\}. \end{aligned}$$

The asymptotic behaviour of the function  $W_0(x)$  at  $x \rightarrow +\infty$  is defined by the factor

$$f(u, v_0) = \frac{\sigma(v_0 - u)}{\sigma(u)} \exp[(u - \omega)\zeta(v_0)],$$

which satisfies the relation

$$f(u + 2n\omega', v_0) = f(u, v_0) \exp[2n\omega'(\zeta(v_0) - \frac{\eta'}{\omega'}v_0)] = f(u, v_0) \exp[2n\omega'k(v_0)].$$

The saddle point  $v_0$  must be chosen in such a manner that the complex number  $\omega'k(v_0)$  has negative real part. From the previous considerations it follows that the point  $\bar{v}_0$  is also a saddle point. The asymptotic behaviour of the function  $W_0(x)$  at  $x \rightarrow -\infty$  is defined by this saddle point which corresponds to the complex number  $\omega'k(\bar{v}_0) = \omega'(\zeta(\bar{v}_0) - (\eta'/\omega')\bar{v}_0)$  with positive real part.  $\square$

It is appropriate to make here some remarks.

According to the theorem

$$W(x) \simeq \exp(-|x||k(\alpha_0)|)|x|^{-3/4}, \quad |x| \rightarrow \infty.$$

It is easy to understand such an asymptotic behaviour of the WF at  $|x| \rightarrow \infty$  if we take into account that

$$W(x) \simeq \operatorname{Re} \left\{ \int_C (k - k_0)^\beta e^{ikx} \right\} \simeq 2 \sin(\beta\pi) \Gamma(1 + \beta) x^{-(1+\beta)} e^{-\Im k_0 x},$$



where  $k_0$  is a branching point of the energy  $E(k)$ , and that, due to a normalization constant of the wave function,

$$\Psi(k) \simeq (k - k_0)^{-1/4},$$

the equality  $\beta = -1/4$  is valid. As far as we know this asymptotic law was mentioned for the first time in [6].

It is of interest to note also that the equation

$$\wp(v) + \frac{\eta'}{\omega'} = 0$$

has obviously the following solution

$$v = \pm \int_{-\frac{\eta'}{\omega'}}^{\infty} \frac{dx}{\sqrt{4x^3 - g_2x - g_3}}.$$

More general problem to solve the equation

$$\wp(v, \omega, \omega') = c(\omega, \omega'),$$

is a well known mathematical problem in the theory of elliptic functions. Solution of the problem in terms of Eisenstein series is presented in the paper[5].

In the above theorem we have obtained results for the Wannier function of lower energy band. Results for the Wannier function of higher band,

(3.26)

$$W(x) = \text{Re} \left\{ -i \frac{\sqrt{-2i\omega'}}{\pi} \int_{\omega}^{\tilde{\omega}} \sqrt{\frac{dk(v)}{dv}} \frac{\sigma(v-u)}{\sigma(v)\sigma(u)} e^{v\eta + (u-\omega)\zeta(v)} dv \right\},$$

$$k(\tilde{\omega}) = \zeta(\tilde{\omega}) - \frac{\eta'}{\omega'} \tilde{\omega} = \frac{\pi}{T},$$

are similar to ones presented above and as a result of that we omit appropriate considerations.

Let us now discuss two limiting cases. The limit  $\tau = \omega'/\omega \rightarrow 0$  corresponds to the free electron case or the empty lattice case. In this limit the energy gap is zero,  $e_1 = e_2$ , there are no saddle points and as a result we have the well known free electron WF

$$W(x) = \frac{T^{1/2}}{\pi x} \sin \left( \frac{\pi x}{T} \right).$$

The limit  $\tau = \omega'/\omega \rightarrow i\infty$  corresponds to the case of tightly bound electrons. In this case the width of the lower energy band is zero,

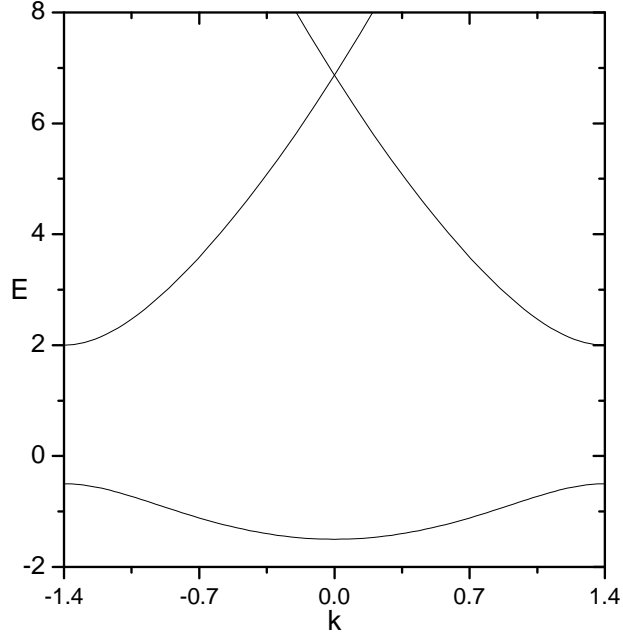


FIGURE 1. Energy bands of the one gap potential with parameters of the elliptic curve  $e_1 = 2, e_2 = -0.5, e_3 = -1.5$

$e_2 = e_3$ , the appropriate wave function looks as follows,

$$\Psi(x) = \left(\frac{\alpha}{2}\right)^{1/2} \frac{1}{\cosh \alpha x}, \quad E_0 = -\alpha^2,$$

where  $E_0$  is the binding energy. The wave functions of higher energy bands are of a form,

$$\Psi(x, k) = \frac{1}{\sqrt{2\pi}\sqrt{k^2 + \alpha^2}} (|k| + i\alpha \tanh(\alpha x)) e^{\pm i k x}, \quad E = k^2.$$

In the next section we shall compare our analytical results with numerical ones.

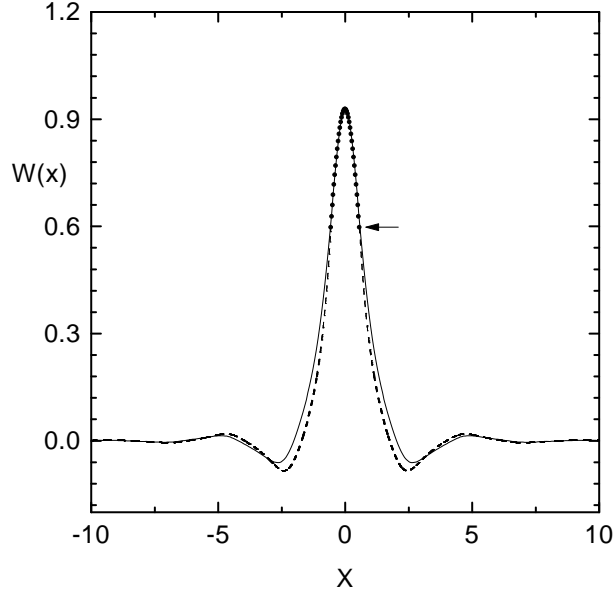


FIGURE 2. The Wannier function associated to the lower band of the one gap potential. The branching points of the elliptic curve are fixed as in Fig. 1. The amplitude of the function in the origin is  $W(0) = 0.93$ . The continuous curve denote the exact expression obtained from numerical calculations, the dashed line corresponds to part of the WF approximated by the asymptotic expansion, while the dotted line denotes the part obtained from the power expansion near the origin. The arrow shows the point where the two different analytical expansions are joined.

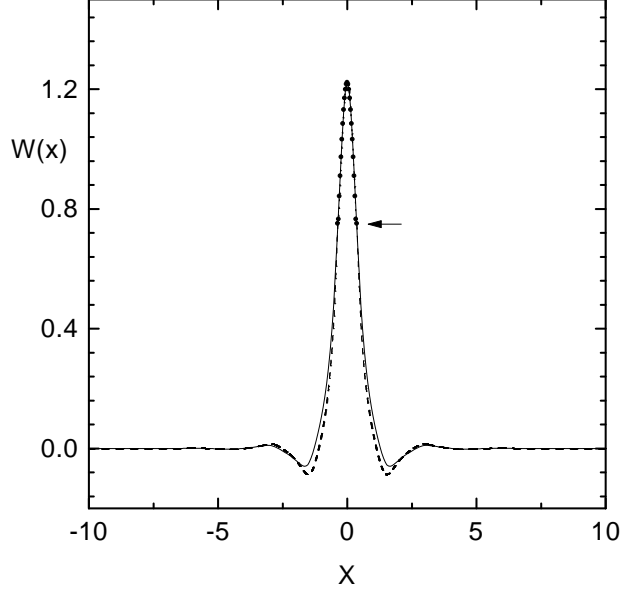


FIGURE 3. Same as in Fig.2 but for a different set of parameters. The branching points of the elliptic curve are  $e_1 = 6, e_2 = -2.0, e_3 = -4.0$ . The value of the function in the origin is  $W(0) = 1.22302$ . The continuous curve denote the exact expression obtained from numerical calculations, the dashed line corresponds to part of the WF approximated by the asymptotic expansion, while the dotted line denotes the part obtained from the power expansion near the origin. The arrow shows the point where the two different analytical expansions are joined.

#### 4. APPROXIMATE ANALYTICAL EXPRESSIONS OF WANNIER FUNCTION AND NUMERICAL RESULTS

The results of the previous section permit to construct the following approximate expression of the WF for one-gap potentials:

$$\begin{aligned}
 W(x) &= W_0 + W_2 x^2 + W_4 x^4 + W_6 x^6, \\
 &\quad \text{for } |x| \leq x_0 \\
 (4.1) \quad &= \text{Re} \left\{ \frac{\sqrt{-2i\omega'}}{\pi} \left( e_1 + \frac{\eta'}{\omega'} \right)^{1/2} \frac{\sigma(v-u)}{\sigma(v)\sigma(u)} \right. \\
 &\quad \times \exp\{(u - \omega)\zeta(v)\} \left[ \frac{i}{2\wp'(v)} \right]^{1/4} \frac{\Gamma(\frac{3}{4})}{x^{\frac{3}{4}}} \Bigg\} \\
 &\quad \text{for } |x| > x_0,
 \end{aligned}$$

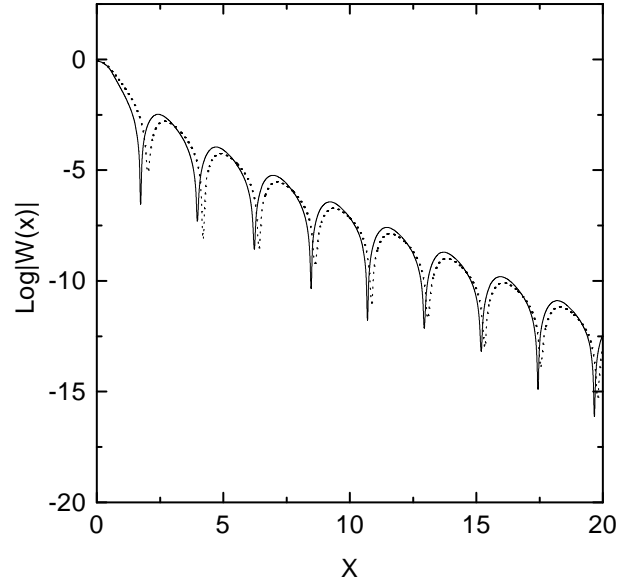


FIGURE 4. Asymptotic decay of the Wannier function in Fig.2 in semi-log scale. The continuous curve represents our analytical approximation while the dotted line is obtained from direct numerical calculations of the WF.

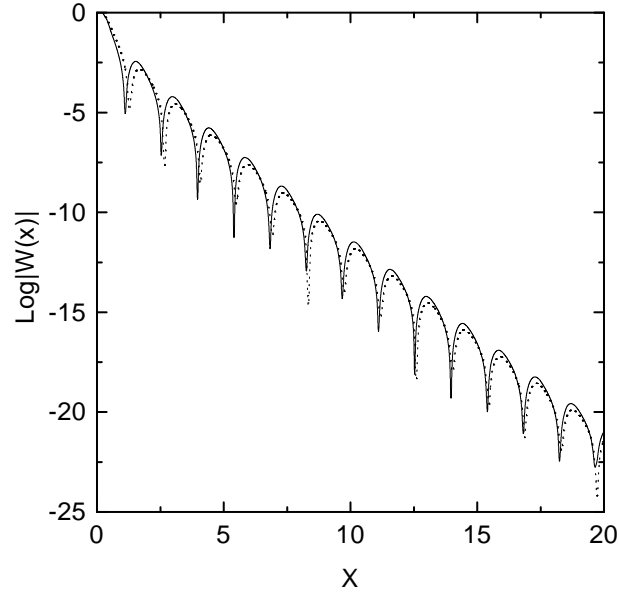


FIGURE 5. Asymptotic decay of the Wannier function in Fig. 3 in semi-log scale. The continuous curve represents our analytical approximation while the dotted line is obtained from direct numerical calculations of the WF.

where  $u = ix + \omega$ ,  $v = v_+ + \omega'$ , the coefficients  $W_0 \dots, W_6$  are given by the formulae (3.8) and the point  $x_0$  is chosen so to satisfy the normalization condition  $\|W(x)\|^2 = 1$ .

To check the validity of this expression we shall compare the WF obtained from Eq.(4.1) with the one obtained directly from the definition (3.1) by numerical methods, using the expression of the normalised BF in Proposition 2.1. In Fig.1 we show the band structure obtained for the one gap potential with parameter values  $e_1 = 2, e_2 = -0.5, e_3 = -1.5$ , while in Fig. 2 we depict the WF associated to the lower band. We see that the agreement between the analytical approximation and direct numerical calculations is excellent both in proximity of the origin and far away from it, these being the regions of validity of the corresponding expansions. In the intermediate region, however, some discrepancy appears. It is possible that for some set of potential parameters the validity regions of the two expansions (near the origin and far from the origin) can overlap at some point  $x_0$  so that it is possible to join them into the single smooth analytical approximation (4.1) which stay close to the exact numerically curve in the whole spatial domain. Existence of the point of such a kind is possible only for one-gap potential. Such a good matching of two expansions is shown in Fig. 3 where the WF of the lower band for a potential with another set of parameters is depicted. By comparing Fig. 3 with Fig. 2 we see that the discrepancy in the intermediate region is smaller for WF which are more localised. This can be understood from the fact that a faster decay of the function (see Figs. 4,5 below) allows the asymptotic expansion to work up to points which are very close to the origin. In Figs. 4 and 5 we show the asymptotic decay of the WF depicted in Figs. 2, 3, respectively from which we see that a stronger localization of the function corresponds to a faster asymptotic decay. The linear decay observed in the semi-log plots of these figures, is fully consistent with the exponential decay of the WF of one-gap elliptic potentials predicted by our analysis.

## 5. CONCLUSIONS

In this paper we have investigated the properties of the Wannier functions of the Schrödinger operator with one gap potentials. As a result we have derived the exact value for the amplitude of the functions in the origin, as well as, an asymptotic expansion characterising the decay of the function at large distances and a power series valid in the vicinity of the origin. Using these expansions we have constructed approximate analytical expressions of the Wannier functions and showed

that they are in good agreement with the ones obtained from numerical results.

We remark that the developed approach can be generalised to the case of finite-gap potentials of more complicated type, like elliptic finite-gap potentials and general finite-gap potentials. We shall discuss these problems in a future publication.

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INSTITUTE OF MAGNETISM, VERNADSKI STR. 36, KIEV-142, UKRAINE, E-MAIL: BEL@IM.IMAG.KIEV.UA

DIPARTIMENTO DI SCIENZE FISICHE "E.R.CAIANIello", VIA S.ALLENDE, 84081 BARONISSI (SA), ITALY, E-MAIL: VZE@MA.HW.AC.UK

DIPARTIMENTO DI SCIENZE FISICHE "E.R.CAIANIello", VIA S.ALLENDE, 84081, BARONISSI (SA), ITALY, E-MAIL: SALERNO@SA.INFN.IT